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Light Water Reactor Sustainability Program

Status Report on the Grizzly Code Enhancements

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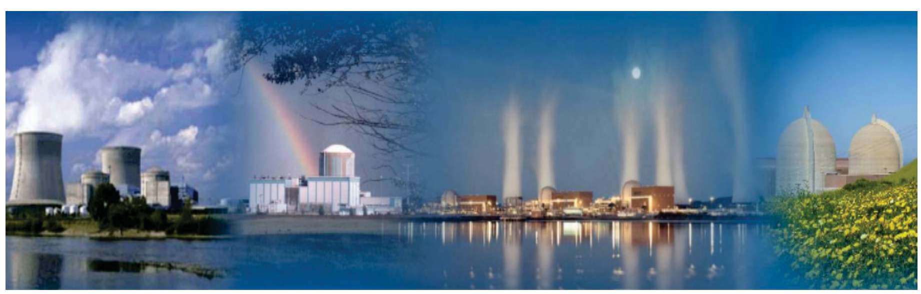
September 2013



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EXECUTIVE SUMMARY

This report summarizes work conducted during fiscal year 2013 to work toward developing a full capability to evaluate fracture contour J-integrals to the Grizzly code. This is a progress report on ongoing work. During the next fiscal year, this capability will be completed, and Grizzly will be capable of evaluating these contour integrals for 3D geometry, including the effects of thermal stress and large deformation. A usable, limited capability has been developed, which is capable of evaluating these integrals on 2D geometry, without considering the effects of material nonlinearity, thermal stress or large deformation. This report presents an overview of the approach used, along with a demonstration of the current capability in Grizzly, including a comparison with an analytical solution.

Status Report on the Grizzly Code Enhancements

1. The J-Integral

Linear elastic fracture mechanics (LEFM) is typically appropriate for fracture assessments of RPVs, and is performed by evaluating stress intensity at a crack location, and comparing that with measures of material toughness, which could include critical stress intensities for crack growth or arrest. The most straightforward method for evaluating the stress intensity is through the *J*-integral [1], the value of which represents the mechanical energy release rate. The *J*-integral is evaluated by performing a surface or volume integral of quantities relating to stress-work density and kinetic energy density per unit volume over a closed contour around the crack tip. The mode-*I* stress intensity factor, K_I, can be directly calculated from the mode-*I* contour integral J_I through the following relationship:

$$K_I = J_I \left(\frac{E}{1 - \nu^2} \right) \tag{1}$$

The ultimate goal of this work is to develop a capability to evaluate *J*-integrals for general 3D cracks to enable fracture assessments of arbitrary crack geometries. During the current year, an initial, limited version of the *J*-integral capability has been developed and demonstrated in Grizzly for 2D small-strain problems, without considering the effects of thermal strain. This development work is in progress, and a full 3D, large deformation capability that includes thermal strain effects will developed in the next year.

Traditionally, *J* is expressed as a surface integral, but it can also be expressed as a volume integral, which lends itself to use in a finite element code. To facilitate implementation of the *J*-integral calculation into the Grizzly finite element program, the method of [2] is employed, in which J_I is represented as:

$$J_I = - \int_V (\mathbf{\Sigma} : \nabla \bar{q}) \, dV \tag{2}$$

where $\boldsymbol{q}$ is a vector field representing contours of virtual displacements at material points due to the virtual extension of the crack front, and $\mathbf{\Sigma}$ is the Eshelby energy-momentum tensor [3], which can be expressed as:

$$\mathbf{\Sigma} = W\boldsymbol{I} - \boldsymbol{F}^T \boldsymbol{P} \tag{3}$$

where W is the stored energy density, $\boldsymbol{I}$ is the identity matrix, $\boldsymbol{F}$ is the deformation gradient, and $\mathbf{P}$ is the first Piola-Kirchoff stress.

The direction of the $\boldsymbol{q}$ vector field used in this form of the integral is constant, but the magnitude of $\boldsymbol{q}$ varies from 1 to 0 based on the distance of a point from the crack tip. Only elements in the region where the magnitude of $\boldsymbol{q}$ is between 0 and 1 contribute to a given contour integral. The user specifies the inner radius of the contour, where the magnitude of the function is 1, and the outer radius, where the magnitude is 0. This concept is applicable to both 2D and 3D models. In a 2D model, a series of concentric contours are defined for the contour integral. In a 3D model, a series of $\boldsymbol{q}$ fields would be defined to calculate the variation of *J* along the crack tip. The magnitudes of these fields would vary in a similar manner to the fields used in 2D, based on distance from the crack tip in a plane normal to the crack, but would also vary based on distance along the crack front. A representative contour plot of the magnitude of $\boldsymbol{q}$ on a 2D finite element domain with a crack tip located at the bottom center of the domain is show in Figure 1.

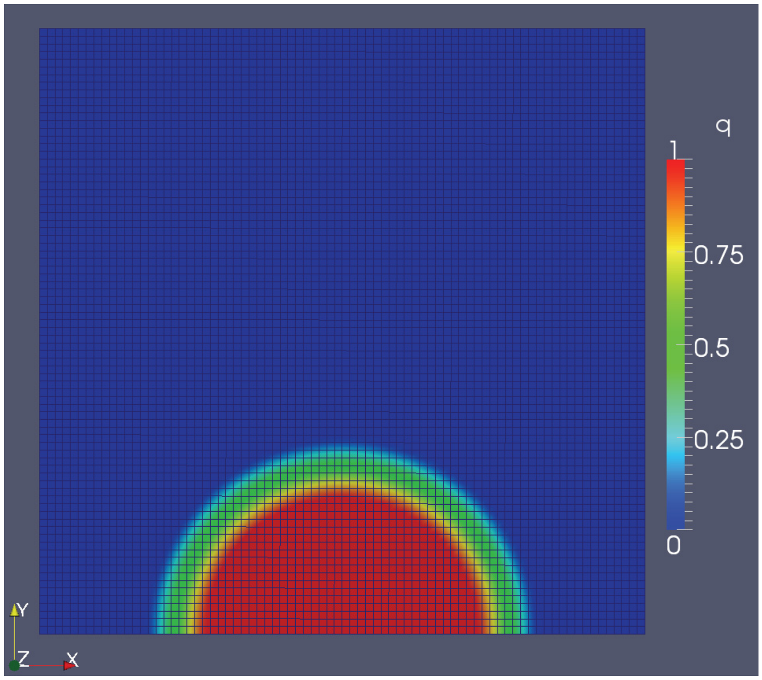

Figure 1. Representative contour plot of the magnitude of $\boldsymbol{q}$ on a 2D domain with a crack tip located at the bottom center of the domain.

The method for evaluating J_I based on equations (2) and (3) was implemented in Grizzly using a combination of code modules that naturally fit within the code environment of MOOSE [5], the framework upon which Grizzly is built. The computation of the value of the of the magnitude of $\boldsymbol{q}$ is done at nodes using a MOOSE AuxKernel, which is a code object that can calculate the value of an arbitrary auxiliary variable at all nodes. The gradient of $\boldsymbol{q}$ is calculated using standard methods available in MOOSE for computing gradients of arbitrary variables at integration points. An option has been added to the base class used for all solid mechanics material models to calculate the Eshelby tensor, $\boldsymbol{\Sigma}$. Finally, a MOOSE PostProcessor, which is a code object that can calculates a single global value based on integration over a domain, performs the integral in equation (2) by summation over the finite elements in the volume integral domain.

To test the *J*-integral calculation in Grizzly, a finite element model of a 2D benchmark problem with a known analytical solution [5] was created and run. The simulation is of a square domain with a center crack. Symmetry boundary conditions were applied at x = 0 and at y = 0 where x > a. A load of 100 N/mm^2 was applied to the top of the domain. Young's modulus = 207GPa and Poisson's ratio of 0.3 were used to define the mechanical properties of the domain. Linear elastic, small displacement, plane strain assumptions were applied and thermal effects ignored. A diagram of this problem is shown in Figure 2.

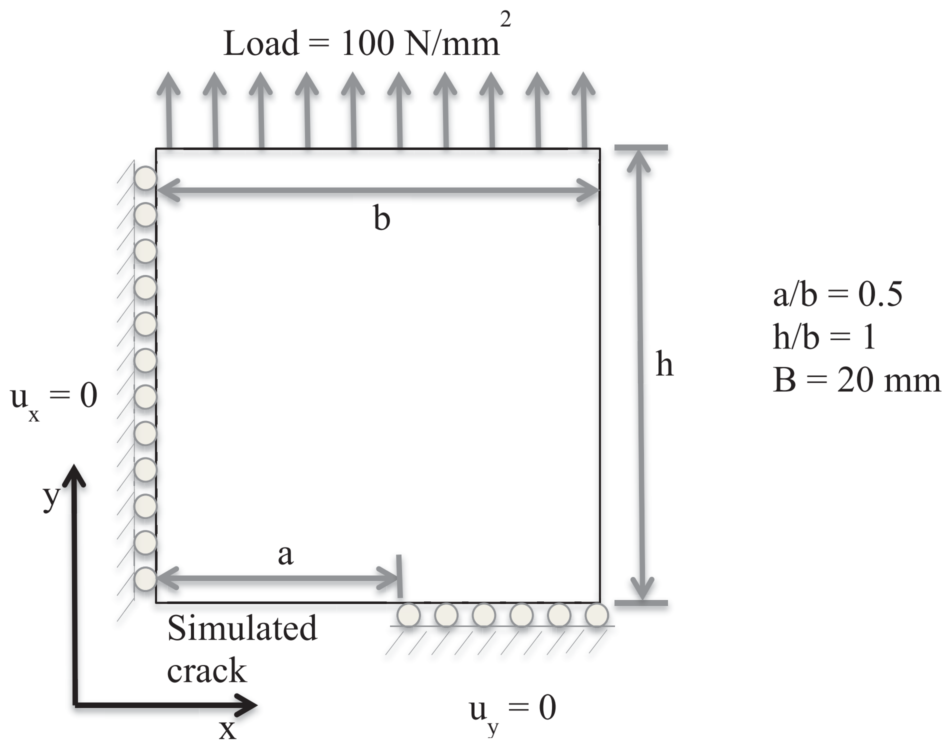

Figure 2. Diagram of 2D benchmark problem.

A contour plot of the displacement field for this problem is shown in Figure 3. Note that the displaced mesh shown in Figure 3 is scaled by a factor of 100 for illustrative purposes.

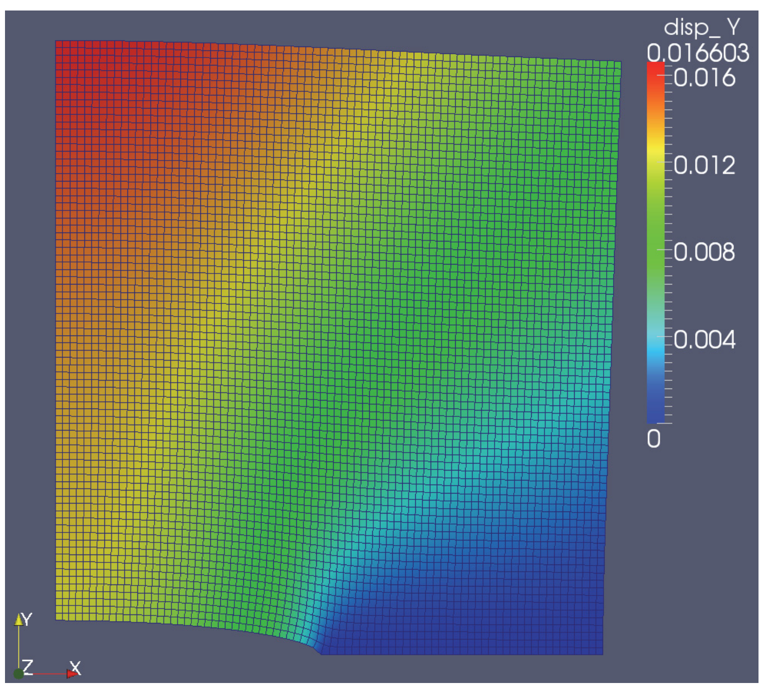

Figure 3. Displacement field for benchmark problem. Note that displaced mesh is magnified by 100 for illustrative purposes.

The analytical (or closed form) solution [5] for this linear elastic fracture mechanics problem is

$$\frac{K_I}{K_0} = 1.325 \tag{3}$$

where

$$\mathbf{K_0} = \sigma\sqrt{\pi a}. \tag{4}$$

and

$$K_I = \sqrt{\frac{J\,E}{1-\upsilon^2}} \tag{5}$$

Solving for *J* with the parameters defined here gives a value of 2.425 for the analytical solution. When calculating *J* numerically, as was done in Grizzly, several *q* functions are defined with different values of inner and outer radii. In this benchmark calculation, we used five *q* functions, with different inner and outer radii (r_i, r_o) values. The values from the Grizzly and analytical calculations of *J* are shown in Table 1. The largest error in the calculated J relative to the analytical solution is 2.9%.

Table 1. Comparison of J values between Grizzly calculations and the analytical solution

(r_i, r_o) values	4, 4.5	4.5, 5	5, 5.5	5.5, 6	6, 6.5
Numerical J	2.455	2.495	2.477	2.428	2.399
Analytical J	2.425				

2. Summary and Future Work

A brief summary of the current progress in implementing a capability to evaluate *J*-integrals in Grizzly, including an overview of the procedure used was presented. A simulation of a benchmark problem with a closed form solution was created and run using Grizzly. The results from the Grizzly numerical calculation and the analytical solution compare favorably.

Assumptions in the current implementation include linear elastic, small displacement, and plane strain 2D behavior. Thermal effects are ignored also. Future development activities are planned to extend the calculation of *J* to three dimensions with large displacements and nonlinear material models including thermal effects.

3. References

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